

ON THE EFFICIENCY OF APPROXIMATE S_N ALBEDO BOUNDARY CONDITIONS FOR MONOENERGETIC X, Y-GEOMETRY CRITICALITY CALCULATIONS

Hermes Alves Filho and Ricardo C. Barros
Departamento de Modelagem Computacional
Instituto Politécnico, IPRJ
Universidade do Estado do Rio de Janeiro, UERJ
Caixa Postal 97282
28601-970 Nova Friburgo, RJ, Brazil

ABSTRACT

We discuss in this paper the efficiency of approximate discrete ordinates (S_N) albedo boundary conditions for one-speed eigenvalue problems in X,Y-geometry. The S_N albedo matrix substitutes approximately the reflector around the multiplying medium, as we neglect the transverse leakage terms within the reflector region. By efficiency we mean analyzing the accuracy of the numerical results versus the CPU execution time of each run of a given model problem. Numerical results to a typical test problem are shown to illustrate this efficiency analysis.

1. INTRODUCTION

It is well known that moderator, reflector and structural materials do not generate power in nuclear reactor cores; therefore we claim we could improve the efficiency of discrete ordinates (S_N) codes for criticality calculations by eliminating the explicit numerical calculations within the non-multiplying regions around the active domain. This can be done by applying albedo boundary conditions, that approximately substitute the reflective properties of the non-active media around the core [1].

In this paper we discuss the efficiency of approximate S_N albedo boundary conditions implemented in a coarse-mesh code, such as the hybrid SD-SGF-CN code [2], and a fine-mesh code, such as the conventional linear diamond (DD) code [3]. By efficiency we mean analyzing the accuracy of the numerical results generated by a computer code for a test problem versus the CPU execution time of each run.

In deriving the S_N albedo matrix, we transverse-integrate the one-speed S_N equations in X,Y geometry inside the reflector region contiguous to the active boundary cell of the spatial grid set up on the domain. That is, for the x direction, we integrate the S_N equations inside the reflector region in the y direction, neglect the transverse leakage terms and solve the resulting homogeneous “one-dimensional” transverse-integrated S_N nodal equations in the x direction analytically by performing a spectral analysis [4]. The procedure follows two major steps: (i) the use of the familiar discretized spatial balance S_N equations [3], with neglect of the leakage terms in the y direction, and (ii) the use of the spectral Green’s function (SGF) auxiliary equations, that have parameters to preserve the analytical general solution of the homogeneous “one-dimensional” transverse integrated S_N nodal equations in the x direction. The procedure for the y direction follows similar steps. Therefore, by substituting the SGF auxiliary equations into the discretized spatial balance S_N equations, we

can relate the neutron angular fluxes backscattered into the active cell to the neutron angular fluxes entering the reflector from the active cell, since vacuum boundary conditions apply on the outer boundaries of the reflector regions.

We remark that the only approximation that we consider in the derivation of the S_N albedo matrices for S_N eigenvalue problems in X,Y geometry is the neglect of the transverse leakage terms. Therefore, should this approximation introduce no significant errors, we expect the use of the present albedo boundary conditions to improve the efficiency of S_N code for criticality calculations, in the sense we have described in this section, except for very coarse-mesh calculations.

At this point, we present an outline of the remainder of this paper. In section 2, we describe how we determine the approximate S_N albedo matrices. In section 3, we show numerical results to a typical model problem, and we list a number of concluding remarks and suggestions for future work in section 4.

2. APPROXIMATE S_N ALBEDO

Let us consider a rectangular spatial grid Ω , where each cell $\Omega_{i,j}$ has width h_i and height k_j , with $i = 1 : (I + 1)$ and $j = 1 : (J + 1)$. Viz Figure 1.

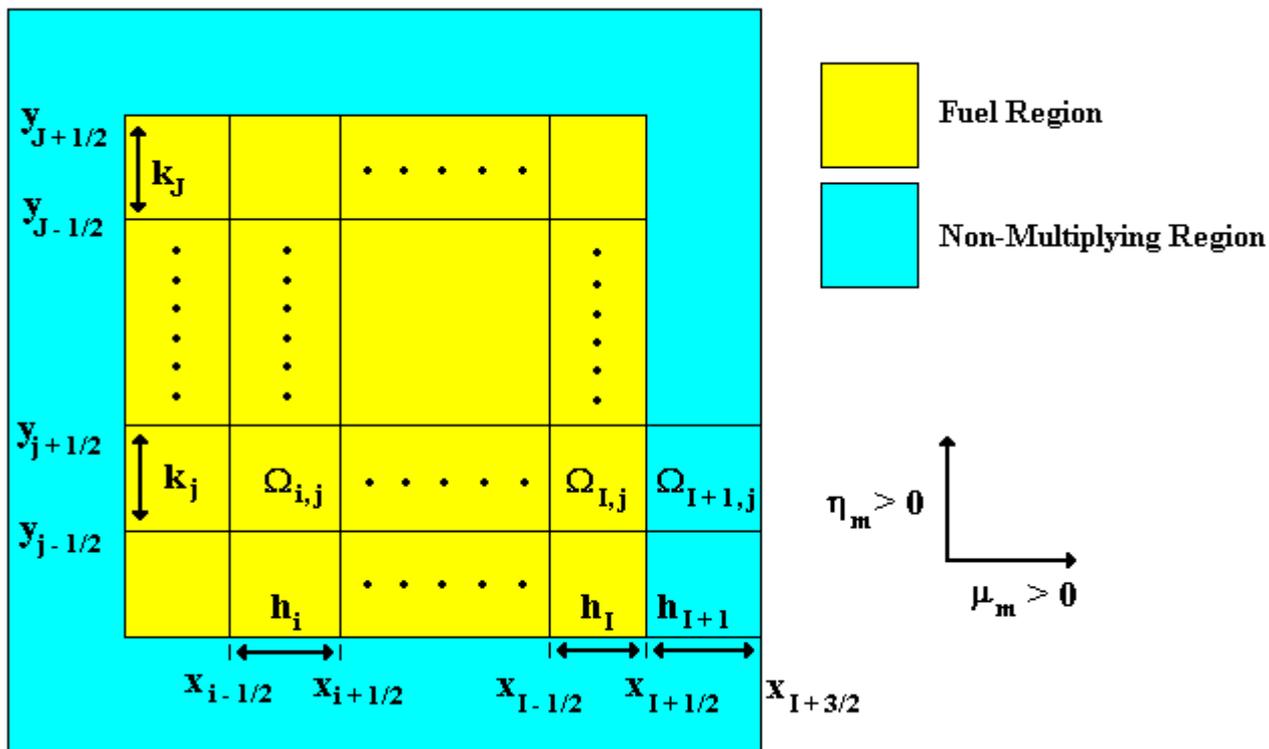


Figure 1. Spatial Grid Ω .

Now, we consider the one-speed S_N equations in X,Y geometry with isotropic scattering

$$\mu_m \frac{\partial}{\partial x} \Psi_m(x, y) + \eta_m \frac{\partial}{\partial y} \Psi_m(x, y) + \sigma_T \Psi_m(x, y) = \sigma_S \sum_{n=1}^M \Psi_m(x, y) w_n, \quad (1)$$

$$m = 1 : M, M = N(N + 2) / 4 .$$

Here the notation is standard [3] and Eq. (1) holds inside a homogeneous non-multiplying medium, e.g., the reflector region around a nuclear reactor core. By integrating Eq.(1) inside an arbitrary node $\Omega_{I+1,j}$ within the reflector, cf. Figure 1, we obtain the familiar discretized spatial balance S_N equations

$$\frac{\mu_m}{h_{I+1}} \left[\tilde{\Psi}_{m,j}(x_{I+3/2}) - \tilde{\Psi}_{m,j}(x_{I+1/2}) \right] + \frac{\eta_m}{k_j} \left[\hat{\Psi}_{m,i}(y_{j+1/2}) - \hat{\Psi}_{m,i}(y_{j-1/2}) \right] + \sigma_{T_{I+1,j}} \bar{\Psi}_{m,I+1,j} = \sigma_{S_{I+1,j}} \sum_{n=1}^M \bar{\Psi}_{n,I+1,j} w_n, \quad m=1:M. \quad (2)$$

where we have used the following definitions:

$\tilde{\Psi}_{m,j}(x)$ = y-direction node-edge average angular flux

$\hat{\Psi}_{m,i}(y)$ = x-direction node-edge average angular flux

$\bar{\Psi}_{m,I+1,j}$ = node-average angular flux.

In order to determine the approximate S_N albedo for the x direction, we neglect the transverse leakage terms in the y direction in Eq. (2) to obtain the “one-dimensional” discretized spatial balance S_N equations

$$\frac{\mu_m}{h_{I+1}} \left[\tilde{\Psi}_{m,j}(x_{I+3/2}) - \tilde{\Psi}_{m,j}(x_{I+1/2}) \right] + \sigma_{T_{I+1,j}} \bar{\Psi}_{m,I+1,j} = \sigma_{S_{I+1,j}} \sum_{n=1}^M \bar{\Psi}_{n,I+1,j} w_n, \quad m=1:M. \quad (3)$$

To proceed further we consider the SGF auxiliary equations

$$\bar{\Psi}_{m,I+1,j} = \sum_{\mu_n > 0} \theta_{m,n} \tilde{\Psi}_{n,j}(x_{I+1/2}) + \sum_{\mu_n < 0} \theta_{m,n} \tilde{\Psi}_{n,j}(x_{I+3/2}), \quad (4)$$

$$m = 1 : M ,$$

where the parameters $\theta_{m,n}$ relate the node-average angular flux within the reflector in a fixed angular direction m to the node-edge average angular fluxes in all the incoming directions. To determine the parameters $\theta_{m,n}$ we first find the expression for the local general solution of the transverse integrated S_N nodal equations in the x direction with neglect of the transverse leakage terms, and then, we substitute it into the SGF auxiliary

equations (4) bearing in mind the average definitions. A detailed description of this procedure can be found in Ref. [5].

Considering that vacuum boundary conditions usually apply on the outer boundaries of the reflector regions for criticality calculations, we simplify the SGF auxiliary equations (4) and substitute them into the “one-dimensional” spatial balance equations (3) to get rid of the node-average angular fluxes. Therefore, we are left with a system of M algebraic linear equations in the y -direction node-edge average angular fluxes *only*.

After some algebra, we write this system in the following matrix compact form

$$\tilde{\Psi}_j \mu_m < 0 (x_{I+1/2}) = \underline{\underline{\Lambda_x}}^R \tilde{\Psi}_j \mu_m > 0 (x_{I+1/2}) , \quad (5)$$

where we have defined

$\underline{\underline{\Lambda_x}}^R =$ approximate S_N albedo matrix to the right hand side boundary of the domain, viz Figure 1

$\tilde{\Psi}_j \mu_m \leq 0 (x_{I+1/2}) = M/2 -$ dimensional vector whose components are the y -direction node-edge average angular at $x_{I+1/2}$ entering the reflector region ($\mu_m > 0$) or entering the fuel region ($\mu_m < 0$).

To obtain the albedo matrices for the left hand side boundary conditions, as well as for the top and bottom, we proceed similarly.

3. NUMERICAL RESULTS

In this section we show numerical results to a test problem that we model using the level symmetric S_4 angular quadrature set [3]. This model problem consists of a heterogeneous critical system, composed of three different material zones, viz Figure 2.

Table I lists the material data for the three zones: two active zones (Pu – 239) and one reflector (water) around the core [6]. Table II displays the numerical results generated for the effective multiplication factor (k_{eff}) by the hybrid SD-SGF-CN method on various spatial grids with both explicit reflector and the approximate S_N albedo boundary conditions. As we see, the use of albedo boundary conditions does not increase significantly the relative deviations with respect to the fine-grid results generated by the conventional DD method with explicit reflector calculation. On the other hand, except for the very coarse spatial grid composed of one node per region (Γ_2 run), the CPU execution time for the albedo calculations decreased with respect to the explicit reflector calculations. As we see, without increasing significantly the relative deviations of the numerical results generated by the SD-SGF-CN method for the eigenvalue k_{eff} with respect to the reference DD result, the albedo calculations reduced the execution time of 13% for the Γ_3 run up to 77% for the Γ_6 run. This is a gain in efficiency in the sense we have described in section 1. Moreover, Table II also shows the results generated for the eigenvalue k_{eff} by the fine-mesh DD method (Γ_8 run) with albedo boundary conditions. We note that the CPU execution time decreased 55% without losing too much accuracy, i.e., the DD run yielded relative deviation of 0.08%, which is comparable to the result generated by the SD-SGF-CN method with albedo boundary

conditions on a spatial grid composed of 8 nodes per region in each spatial direction (Γ_5 run, 33.180 seconds).

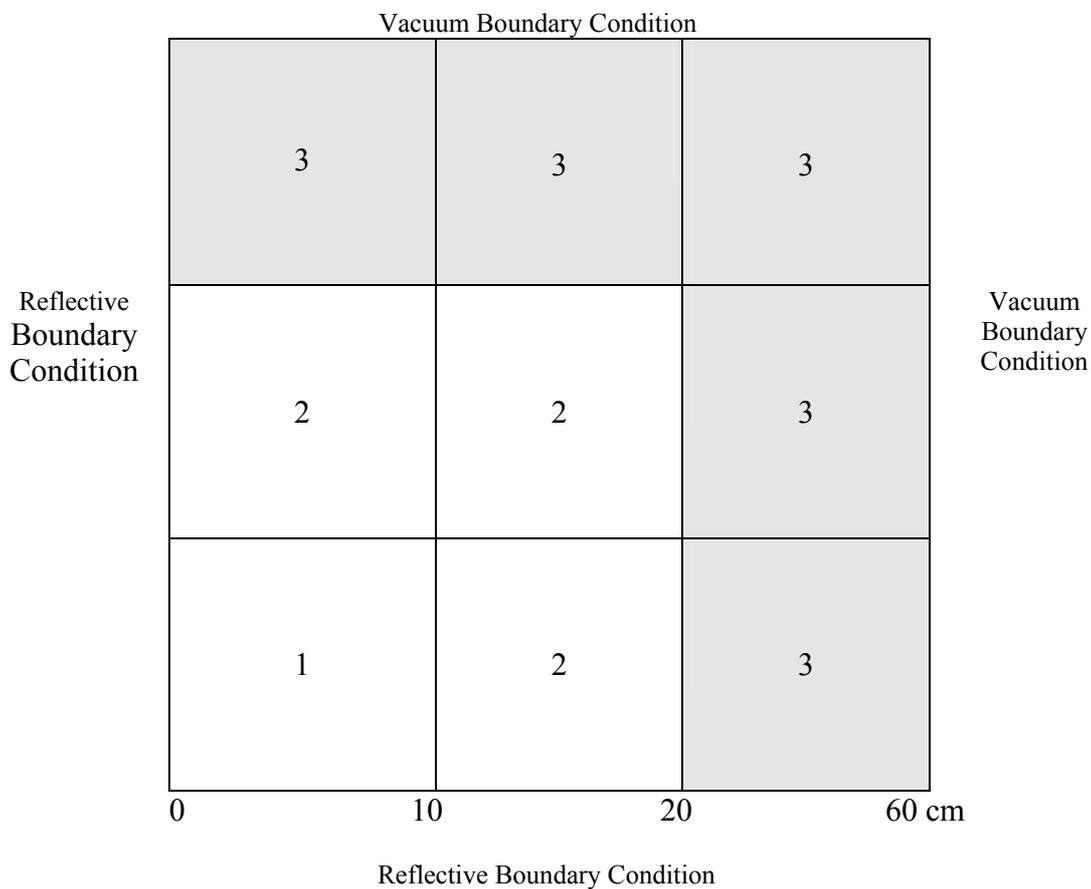


Figure 2. Test Problem (critical system, $k_{\text{eff}} = 1.0$).

Table I. Material data to the Test Problem.

Zone Number	σ_T	σ_S	$\nu\sigma_F$
1	3.26400E-1 ^a	2.25216E-1	0.11491E+0
2	3.26400E-1	2.25216E-1	0.10072E+0
3	3.26400E-1	2.93760E-1	0.0

^a Read as 3.26400×10^{-1} .

Table II. Numerical Results for the Test Problem.

Spatial Grid Γ_n^a	Numerical Method	Dominant Eigenvalue (k_{eff})	Relative Deviation (%) f	CPU time (seconds)	CPU time reduction (%)
Γ_2	SD-SGF-CN ^b	1.00382542	0.38	7.240	-
	SD-SGF-ALB ^c	1.00401558	0.40	7.790	
Γ_3	SD-SGF-CN	1.00142256	0.14	14.490	13
	SD-SGF-ALB	1.00179353	0.18	12.600	
Γ_4	SD-SGF-CN	1.00048247	0.05	25.640	30
	SD-SGF-ALB	1.00105290	0.10	18.040	
Γ_5	SD-SGF-CN	1.00011536	0.01	55.800	40
	SD-SGF-ALB	1.00084038	0.08	33.180	
Γ_6	SD-SGF-CN	1.00005177	0.00	812.960	77
	SD-SGF-ALB	1.00078486	0.08	187.030	
Γ_8	DD-CBI ^d	1.00001189	-	2545.380	55
	DD-ALB ^e	1.00076461	0.08	1137.220	

^a $2^n / 4$ spatial nodes per region in each spatial direction.

^b Spectral diamond-spectral Green's function-constant nodal method with explicit reflector.

^c Spectral diamond-spectral Green's function-constant nodal method with albedo boundary conditions.

^d Diamond difference method with explicit reflector (reference result).

^e Diamond difference method with albedo boundary conditions.

^f Relative deviation with respect to the DD fine-mesh solution.

Supposing that the power density generated by the entire domain is 1 Watt/cm³, Figure 3 shows the power density distribution as generated by four independent runs: the fine-grid explicit reflector and albedo DD runs on a spatial grid composed of 64 cells per region in each spatial direction (Γ_8); and the coarse-grid explicit reflector and albedo SD-SGF-CN runs on a spatial grid composed of one node per region (Γ_2). As we see in Figure 4, the relative deviations for this numerical experiment are acceptable for practical applications.

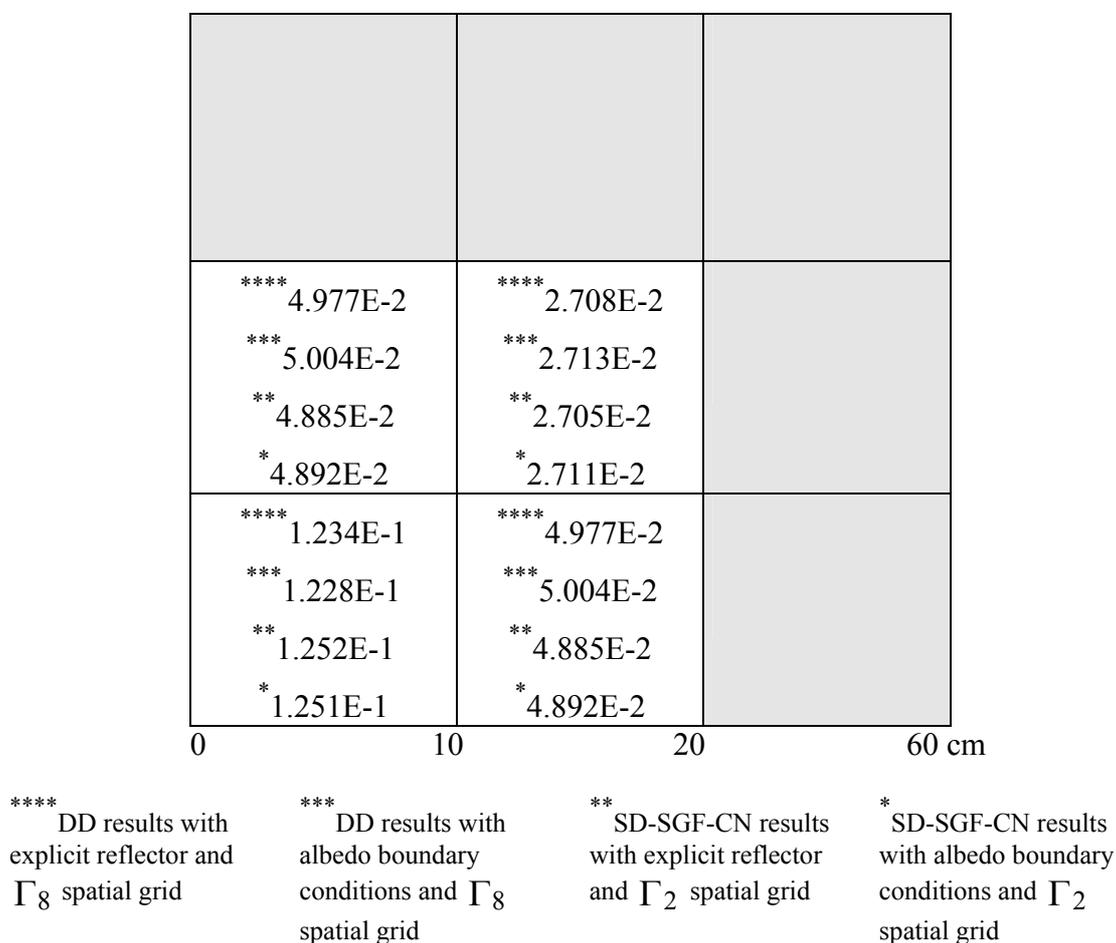


Figure 3. Power Density Distribution for the Test Problem.

*** 0.53 ** 1.72 * 1.85	*** 0.20 ** 0.06 * 0.08	
*** 0.48 ** 1.36 * 1.51	*** 0.53 ** 1.72 * 1.85	
0	10	20
		60 cm

*** DD results with albedo boundary conditions and Γ_8 spatial grid

** SD-SGF-CN results with explicit reflector and Γ_2 spatial grid

* SD-SGF-CN results with albedo boundary conditions and Γ_2 spatial grid

Figure 4. Relative Deviation (%) in Power Density Distribution for the Test Problem.

4. CONCLUDING REMARKS

Based on the numerical experiments described in the previous section, we list a number of general conclusions and suggestions for future work:

- the approximate S_N albedo boundary conditions for criticality calculations substitute very accurately the reflector around the active core;
- without losing too much accuracy, the use of albedo boundary conditions reduced significantly the CPU execution time of each run. This is particularly noticeable for fine-grid calculations.
- the S_N albedo boundary conditions, as described in this paper, can be implemented in various conventional numerical methods for one-speed X,Y-geometry S_N criticality calculations, such as the linear diamond method, the step-characteristic method and the discontinuous finite element methods;
- we are now working on the approximate S_N albedo boundary conditions for multilayer non-multiplying regions around the active core, e.g., baffle-reflector system. We intend to report on the results when they are fully tested;
- for practical applications in nuclear reactor global calculations, the multigroup approximate S_N albedo boundary conditions are of great interest to account for the neutron energy change in nuclear interactions. This is another suggestion for future work.

ACKNOWLEDGMENTS

This work was sponsored by CNPq and FAPERJ – Brazil.

REFERENCES

1. H. Alves Filho and R. C. Barros, “Discrete Ordinates Albedo Boundary Conditions for One-Speed Eigenvalue Problems in X, Y Geometry”, *Proceedings of the 2001 International Meeting on Mathematical Methods for Nuclear Applications*, September 09-13, 2001, Salt Lake City, Utah, USA, CD-ROM (2001).
2. H. Alves Filho, R.C. Barros and F.C. da Silva, “The Hybrid Spectral Diamond-Spectral Green’s Function-Constant Nodal Method for One-Speed X,Y-Geometry S_N Eigenvalue Problems”, *Proceedings of the International Conference on Mathematics and Computation, Reactor Physics and Environmental Analyses*, Vol. 2, Madrid, pp. 1608-1617 (1999).
3. E.E. Lewis and W.F. Miller Jr, *Computational Methods of Neutron Transport*, American Nuclear Society, La Grange Park, Illinois, USA (1984).
4. R.C. Barros, H. Alves Filho and F.C. da Silva, “Recent Advances in Spectral Nodal Methods for X,Y-Geometry Discrete Ordinates Deep Penetration and Eigenvalue Problems”, *Progress in Nuclear Energy*, **35**, pp. 293-331 (1999).
5. R.C. Barros and E.W. Larsen, “A Spectral Nodal Method for One-Group X, Y-Geometry Discrete Ordinates Problems”, *Nuclear Science and Engineering*, **111**, pp. 34-45 (1992).
6. A. Sood, R. A. Forster and D. K. Parsons, “Analytical Benchmark Test Set for Criticality Code Verification”, LA-13511 (1999).